WWU
MÜNSTER

A certified and adaptive RB-ML-ROM surrogate approach for parametrized PDEs

Young Mathematicians in Model Order Reduction – YMMOR

Bernard Haasdonk, Hendrik Kleikamp, Mario Ohlberger,
Felix Schindler, Tizian Wenzel

July 18 – 22, 2022

living.knowledge

MM
Mathematics
Münster
Cluster of Excellence

Setting

Parametrized parabolic PDE in weak form: Find $u(\mu) \in L^2(0,T;V)$ s.t.

$$\begin{aligned} \langle \partial_t u(\mu), v \rangle + a(u(\mu), v; \mu) &= l(v;\mu), && \text{for all } v \in V, \\ u(0;\mu) &= u_0(\mu), && \text{for } u_0(\mu) \in V, \end{aligned}$$

with coercive bilinear form a, linear functional l and initial condition u_0.

Setting

Parametrized parabolic PDE in weak form: Find $u(\mu) \in L^2(0,T;V)$ s.t.

$$\begin{aligned} \langle \partial_t u(\mu), v \rangle + a(u(\mu), v; \mu) &= l(v;\mu), && \text{for all } v \in V, \\ u(0;\mu) &= u_0(\mu), && \text{for } u_0(\mu) \in V, \end{aligned}$$

with coercive bilinear form a, linear functional l and initial condition u_0.

Examples later on:

- PDE-constrained optimization / inverse problem.
- Monte Carlo estimation of quantity of interest.

Setting

Parametrized parabolic PDE in weak form: Find $u(\mu) \in L^2(0,T;V)$ s.t.

$$\begin{aligned} \langle \partial_t u(\mu), v \rangle + a(u(\mu), v; \mu) &= l(v;\mu), && \text{for all } v \in V, \\ u(0;\mu) &= u_0(\mu), && \text{for } u_0(\mu) \in V, \end{aligned}$$

with coercive bilinear form a, linear functional l and initial condition u_0.

Examples later on:

- PDE-constrained optimization / inverse problem.
- Monte Carlo estimation of quantity of interest.

Need for Model Order Reduction!

Reduced basis (RB) reduced order models

- Build reduced space $V_N \subset V_h$ with $N := \dim V_N \ll \dim V_h$ (e.g. using Greedy algorithm, POD, HaPOD,...).
- Perform Galerkin projection onto V_N instead of V_h.
- Full offline-online-decomposition under certain assumptions on parameter dependence of a and l.
- Solve small linear system in each time step t_k for the coefficients $u_{\mathrm{RB}}(\mu; t_k) \in \mathbb{R}^N$ with respect to the basis $\varphi_1, \dots, \varphi_N$ of V_N.
- Reconstruct approximate solution by linear combination of $\varphi_1, \dots, \varphi_N$.

Reduced basis (RB) reduced order models

- Build reduced space $V_N \subset V_h$ with $N := \dim V_N \ll \dim V_h$ (e.g. using Greedy algorithm, POD, HaPOD,...).
- Perform Galerkin projection onto V_N instead of V_h.
- Full offline-online-decomposition under certain assumptions on parameter dependence of a and l.
- Solve small linear system in each time step t_k for the coefficients $u_{\mathrm{RB}}(\mu; t_k) \in \mathbb{R}^N$ with respect to the basis $\varphi_1, \dots, \varphi_N$ of V_N.
- Reconstruct approximate solution by linear combination of $\varphi_1, \dots, \varphi_N$.

Reduced basis (RB) reduced order models

- Build reduced space $V_N \subset V_h$ with $N := \dim V_N \ll \dim V_h$ (e.g. using Greedy algorithm, POD, HaPOD,...).
- Perform Galerkin projection onto V_N instead of V_h.
- Full offline-online-decomposition under certain assumptions on parameter dependence of a and l.
- Solve small linear system in each time step t_k for the coefficients $u_{\mathrm{RB}}(\mu; t_k) \in \mathbb{R}^N$ with respect to the basis $\varphi_1, \dots, \varphi_N$ of V_N.
- Reconstruct approximate solution by linear combination of $\varphi_1, \dots, \varphi_N$.

Reduced basis (RB) reduced order models

- Build reduced space $V_N \subset V_h$ with $N := \dim V_N \ll \dim V_h$ (e.g. using Greedy algorithm, POD, HaPOD,...).
- Perform Galerkin projection onto V_N instead of V_h.
- Full offline-online-decomposition under certain assumptions on parameter dependence of a and l.
- Solve small linear system in each time step t_k for the coefficients $u_{\mathsf{RB}}(\mu; t_k) \in \mathbb{R}^N$ with respect to the basis $\varphi_1, \dots, \varphi_N$ of V_N.
- Reconstruct approximate solution by linear combination of $\varphi_1, \dots, \varphi_N$.

Reduced basis (RB) reduced order models

- Build reduced space $V_N \subset V_h$ with $N := \dim V_N \ll \dim V_h$ (e.g. using Greedy algorithm, POD, HaPOD,...).
- Perform Galerkin projection onto V_N instead of V_h.
- Full offline-online-decomposition under certain assumptions on parameter dependence of a and l.
- Solve small linear system in each time step t_k for the coefficients $u_{\mathsf{RB}}(\mu; t_k) \in \mathbb{R}^N$ with respect to the basis $\varphi_1, \dots, \varphi_N$ of V_N.
- Reconstruct approximate solution by linear combination of $\varphi_1, \dots, \varphi_N$.

Machine learning surrogate models

- Learn map from parameter $\mu \in \mathcal{P}$ to coefficients $\underline{u_{\mathsf{RB}}(\mu; t_k)} \in \mathbb{R}^N$ using machine learning, e.g. kernel models or neural networks.

Machine learning surrogate models

- Learn map from parameter $\mu \in \mathcal{P}$ to coefficients $u_{\mathrm{RB}}(\mu; t_k) \in \mathbb{R}^N$ using machine learning, e.g. kernel models or neural networks.
- Two different approaches:
  - *Time-"vectorized":* Train $\Phi \colon \mathbb{R}^p \to \mathbb{R}^{K \times N}$, with $p := \dim \mathcal{P}$ and K the number of time steps, to predict the ROM coefficients for all time steps at once.
  - *"Random-access"-in-time:* Train $\Phi \colon \mathbb{R}^{p+1} \to \mathbb{R}^N$ to predict the ROM coefficients at any point in time. (similar to [Wang/Hesthaven/Ray'19])

Machine learning surrogate models

- Learn map from parameter $\mu \in \mathcal{P}$ to coefficients $u_{\mathsf{RB}}(\mu; t_k) \in \mathbb{R}^N$ using machine learning, e.g. kernel models or neural networks.
- Two different approaches:
  - *Time-"vectorized":* Train $\Phi \colon \mathbb{R}^p \to \mathbb{R}^{K \times N}$, with $p := \dim \mathcal{P}$ and K the number of time steps, to predict the ROM coefficients for all time steps at once.
  - *"Random-access"-in-time:* Train $\Phi \colon \mathbb{R}^{p+1} \to \mathbb{R}^N$ to predict the ROM coefficients at any point in time. (similar to [Wang/Hesthaven/Ray'19])
- Obtain DoF-vector $u_{\mathsf{ML}}(\mu; t_k) \in \mathbb{R}^N$ and corresponding solution $u_{\mathsf{ML}}(\mu; t_k) \in V_N$ by evaluating Φ for parameter $\mu \in \mathcal{P}$.

Comparison of the models

Full-order/high-fidelity model (FOM)

Pros:

- arbitrarily accurate solutions

Cons:

- very slow when considering fine discretizations and many time steps

Comparison of the models

Full-order/high-fidelity model (FOM)

Pros:

- arbitrarily accurate solutions

Cons:

- very slow when considering fine discretizations and many time steps

Reduced order model (ROM)

Pros:

- faster than FOM
- error estimator

Cons:

- slow iterative time stepping
- solve dense linear system in each time step

Comparison of the models

Full-order/high-fidelity model (FOM)

Pros:

- arbitrarily accurate solutions

Cons:

- very slow when considering fine discretizations and many time steps

Reduced order model (ROM)

Pros:

- faster than FOM
- error estimator

Cons:

- slow iterative time stepping
- solve dense linear system in each time step

Machine learning model (MLM)

Pros:

- faster than ROM
- parallel evaluation for different time instances

Cons:

- no certification available (so far)

Parabolic RB a posteriori error estimator [Grepl/Patera'05]

Offline-online-decomposable error estimate for difference between FOM-solution $u_h(\mu) \in V_h$ and ROM-solution $u_{\mathsf{RB}}(\mu) \in V_N$:

$$\|u_h(\mu) - u_{\mathsf{RB}}(\mu)\|_{L^2(0,T;V_h)} \leq E_{\mathsf{RB}}(u_{\mathsf{RB}}(\mu);\mu)$$

$$:= \underbrace{\alpha(\mu)}_{\substack{\text{coercivity}\\ \text{constant}}}^{-1} \left(\sum_{k=1}^{K-1} \Delta t \| \underbrace{R_k(u_{\mathsf{RB}}(t_k;\mu);\mu)}_{\substack{\text{residuum in the}\\ k\text{-th time step}}} \|_{V_h'}^2 \right)^{1/2}$$

Parabolic RB a posteriori error estimator [Grepl/Patera'05]

Offline-online-decomposable error estimate for difference between FOM-solution $u_h(\mu) \in V_h$ and ROM-solution $u_{\mathsf{RB}}(\mu) \in V_N$:

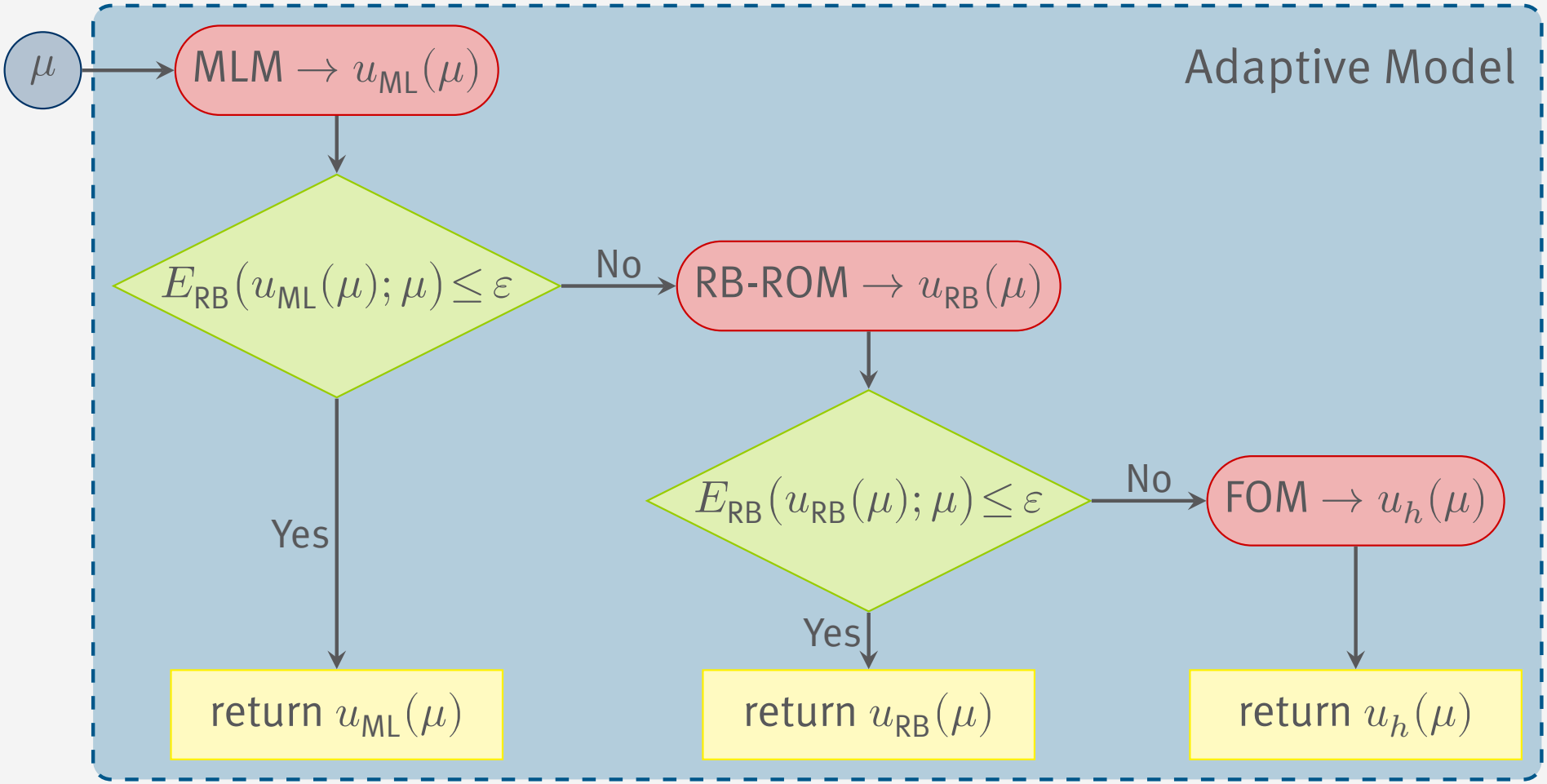
$$\|u_h(\mu) - u_{\mathsf{RB}}(\mu)\|_{L^2(0,T;V_h)} \leq E_{\mathsf{RB}}(u_{\mathsf{RB}}(\mu);\mu)$$

$$:= \underbrace{\alpha(\mu)}_{\substack{\text{coercivity}\\ \text{constant}}}^{-1} \left(\sum_{k=1}^{K-1} \Delta t \| \underbrace{R_k(u_{\mathsf{RB}}(t_k;\mu);\mu)}_{\substack{\text{residuum in the}\\ k\text{-th time step}}} \|_{V_h'}^2 \right)^{1/2}$$

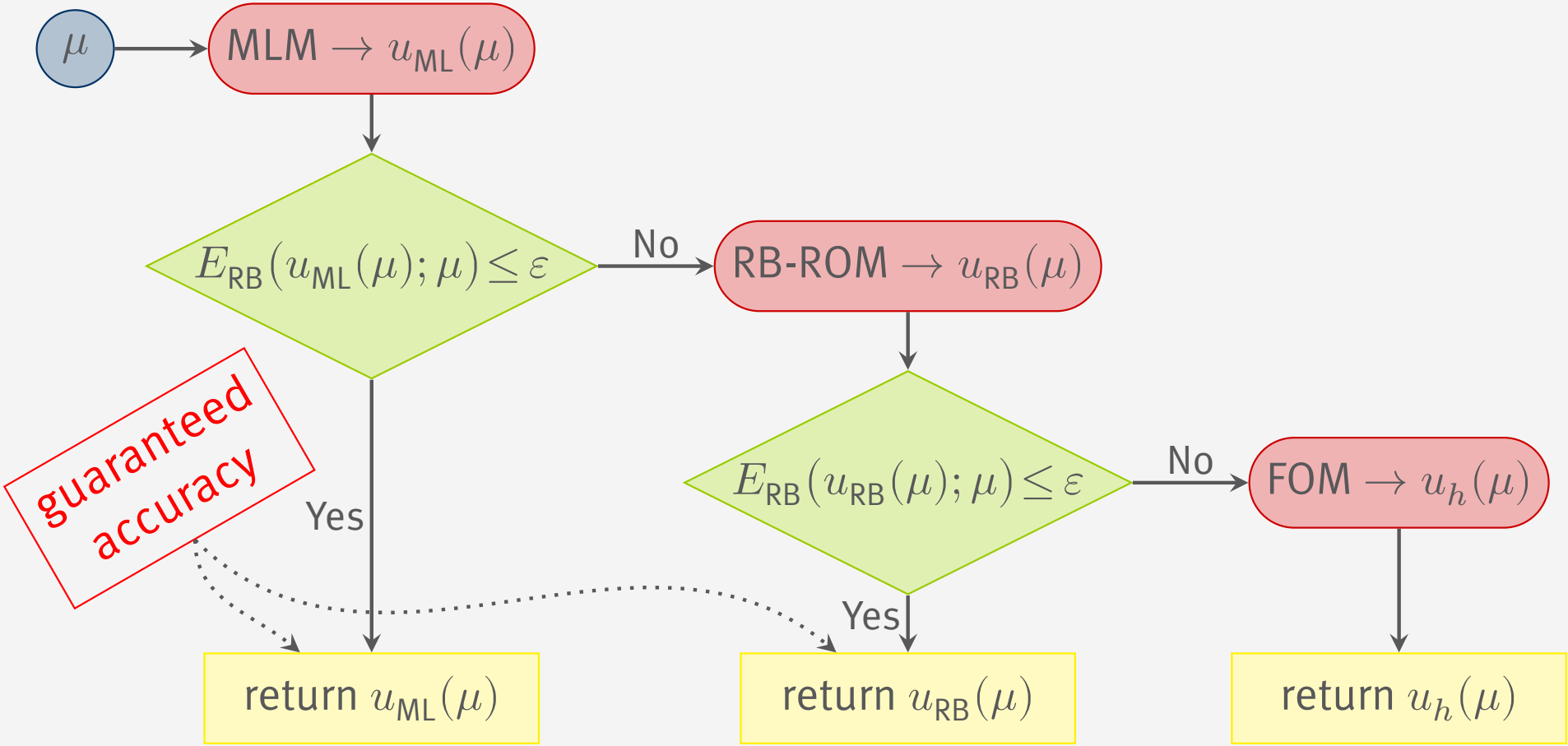
Idea: Apply error estimator E_{RB} to machine learning prediction $u_{\mathsf{ML}}(\mu)$!

$\Longrightarrow$ A posteriori certification of machine learning results!

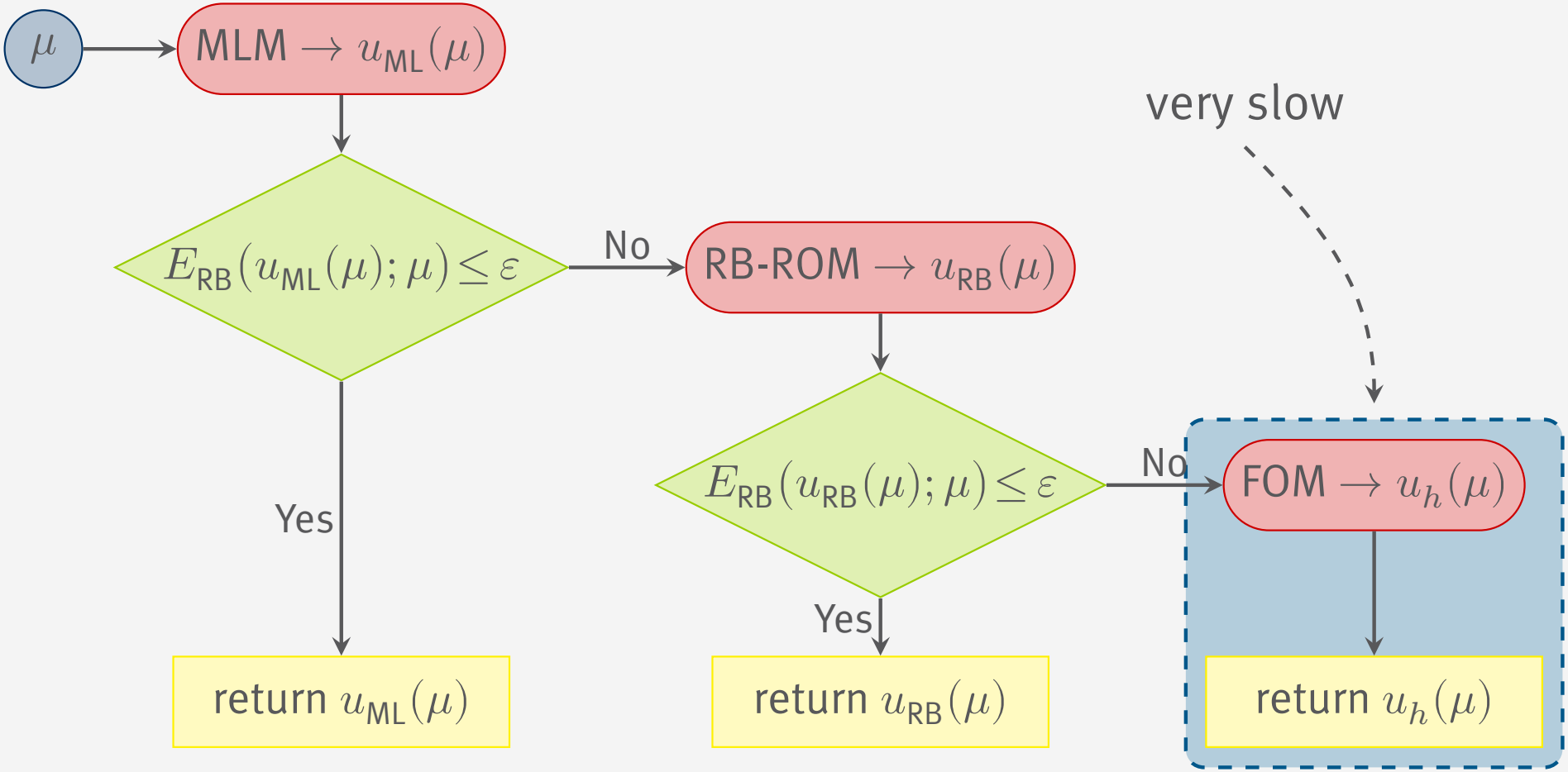
Adaptive model hierarchy [Haasdonk et al'22]



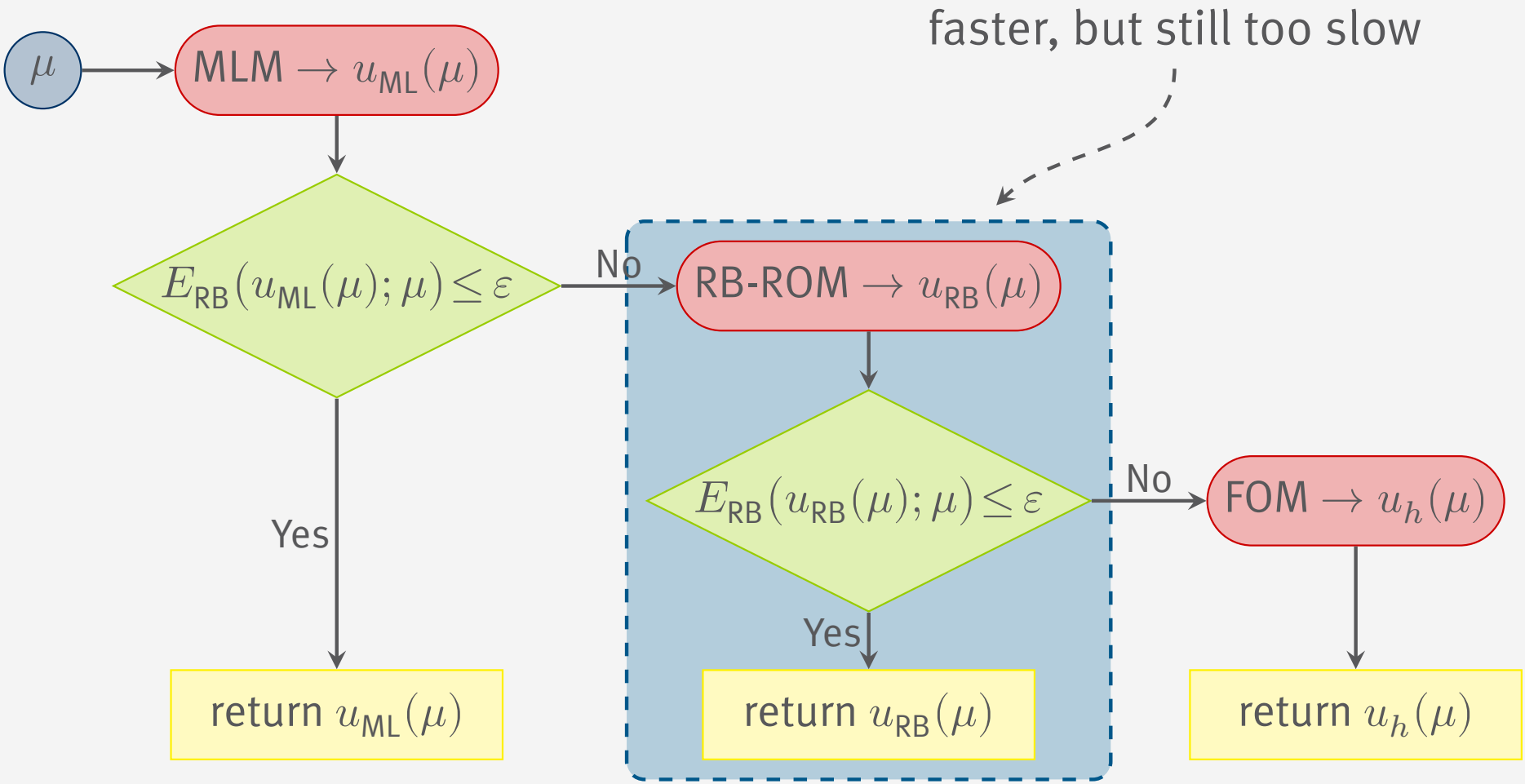
Adaptive model hierarchy [Haasdonk et al'22]



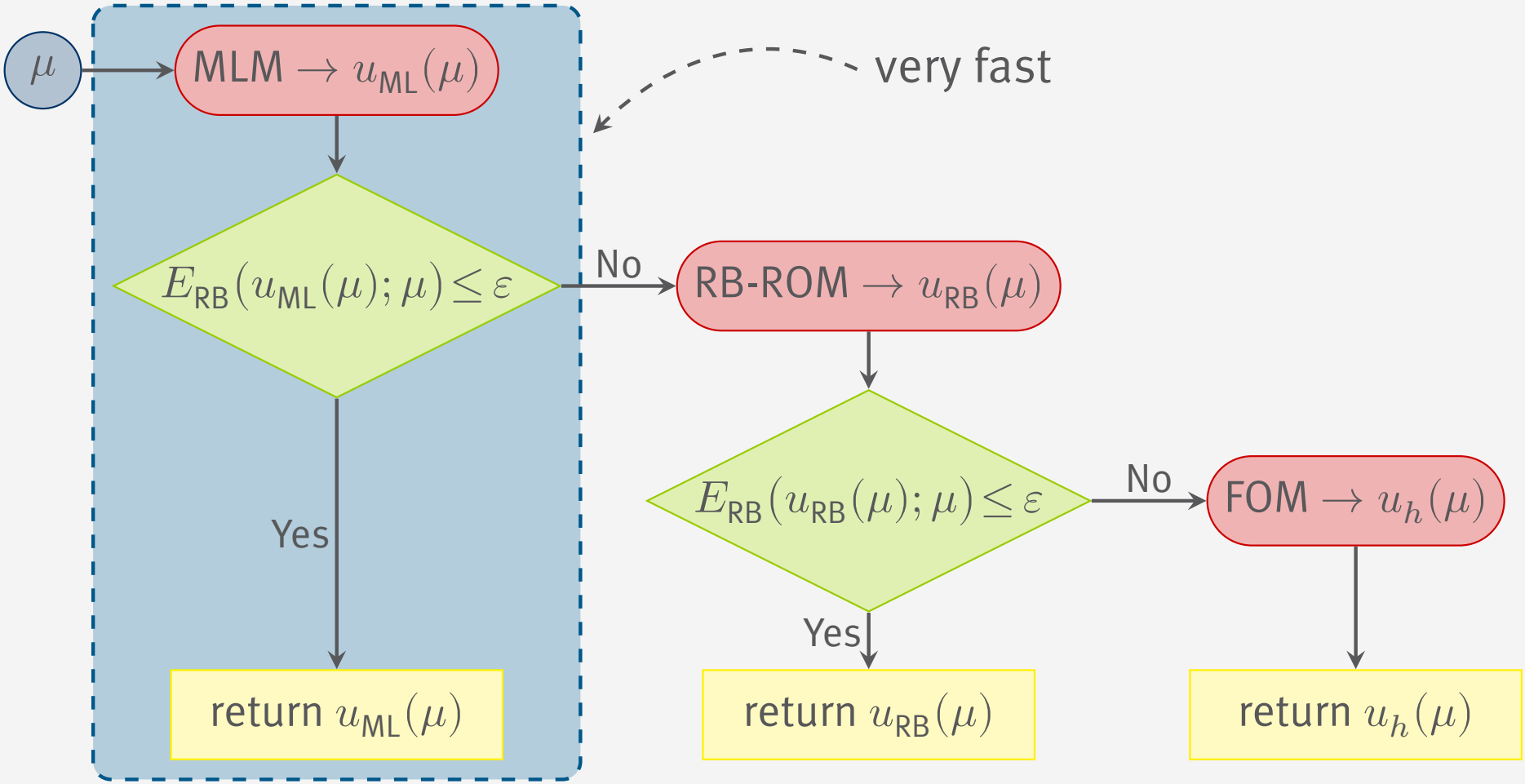
Adaptive model hierarchy [Haasdonk et al'22]



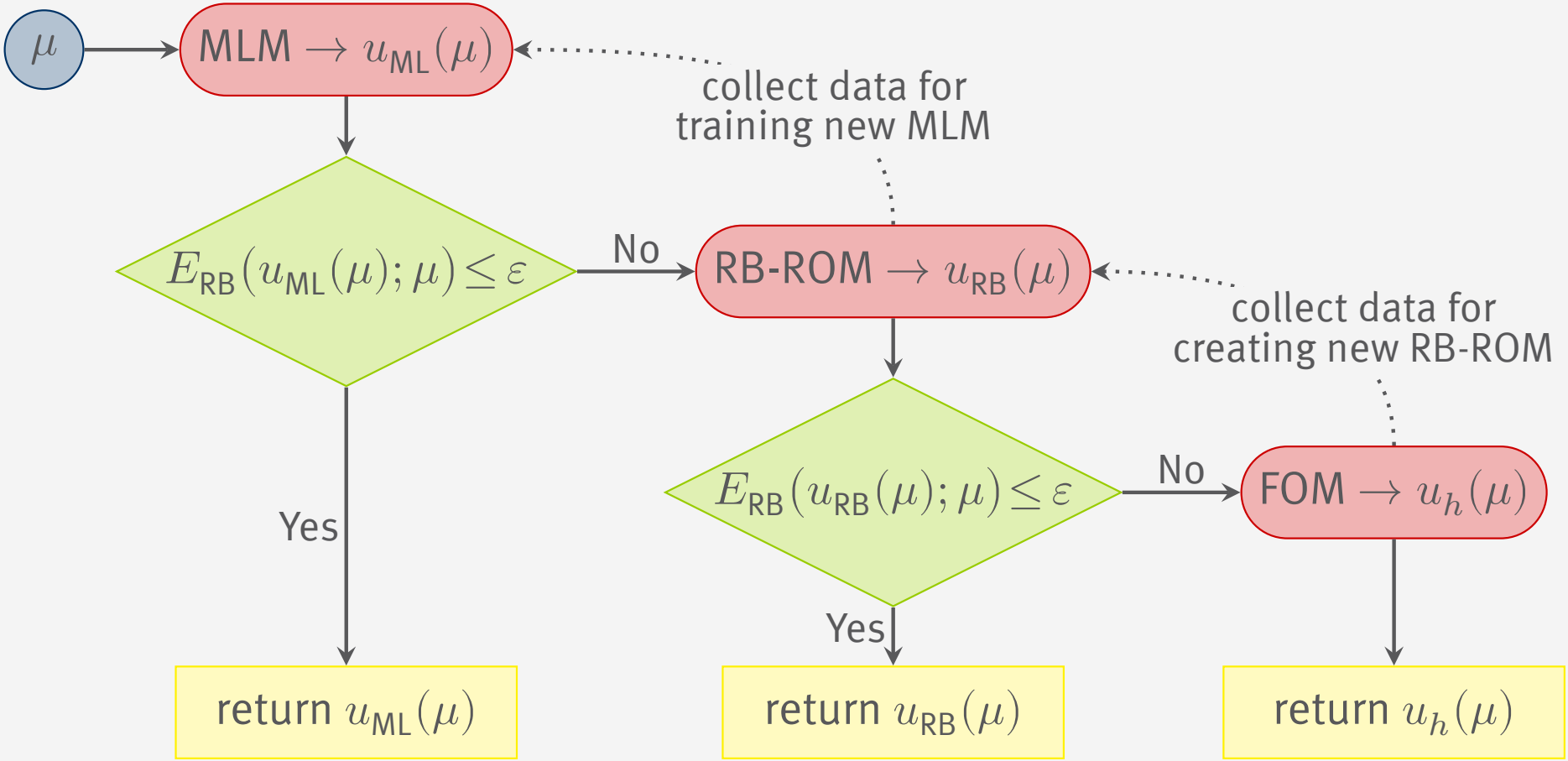
Adaptive model hierarchy [Haasdonk et al'22]



Adaptive model hierarchy [Haasdonk et al'22]



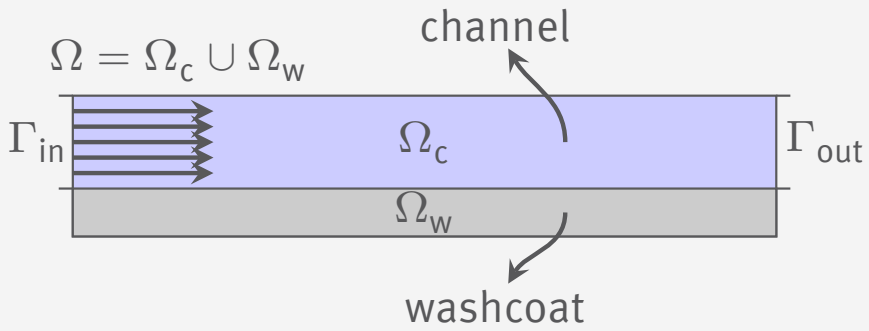
Adaptive model hierarchy [Haasdonk et al'22]



Numerical experiments I – PDE-constr. optimization

Advection-diffusion-reaction with $\mu = (\mathrm{Da}, \mathrm{Pe}) \in \mathcal{P} = [0.01, 10] \times [9, 11]$:

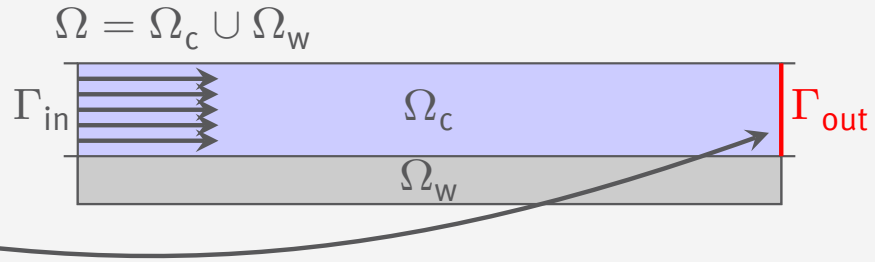
$$
\begin{aligned}
\partial_t u(\mu) - \nabla \cdot (\kappa \nabla u(\mu)) + \mathrm{Pe}\, \nabla \cdot (\vec{v}\, u(\mu)) + \mathrm{Da}\, \chi_{\Omega_w} u(\mu) = 0 \quad & \text{in } \Omega \times (0, T), \\
(\kappa \nabla u(\mu)) \cdot n_{\partial\Omega} = 0 \quad & \text{on } \Gamma_{\text{out}}, \\
u(\mu) = \chi_{\Gamma_{\text{in}}} \quad & \text{on } \partial\Omega \backslash \Gamma_{\text{out}}, \\
u(t = 0; \mu) = \chi_{\Gamma_{\text{in}}} \quad & \text{in } \Omega.
\end{aligned}
$$



Numerical experiments I – PDE-constr. optimization

Break-through curve as output functional:

$$f(t;\mu) = \frac{1}{|\Gamma_{\text{out}}|} \int_{\Gamma_{\text{out}}} u(t;\mu)\,\mathrm{d}s$$



PDE-constrained optimization problem:

$$\min_{\mu\in\mathcal{P}} \mathcal{J}(\mu) := \|\hat{f}_h - f_{\text{adapt}}(\mu)\|_{L^\infty([0,T])}$$

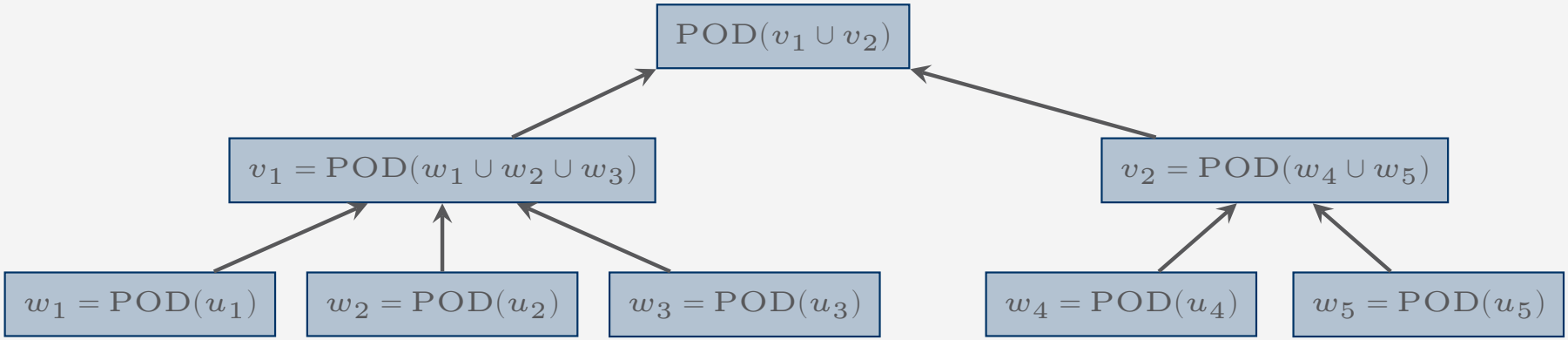
Here, $\hat{f}_h = f_h(\hat{\mu})$ is a desired break-through curve with $\hat{\mu} = (5.005, 10)$.

Goal: Find the parameter $\mu \in \mathcal{P}$ that produces the break-through curve $\hat{f}_h$ (can be seen as an inverse problem).

Numerical experiments I – PDE-constr. optimization

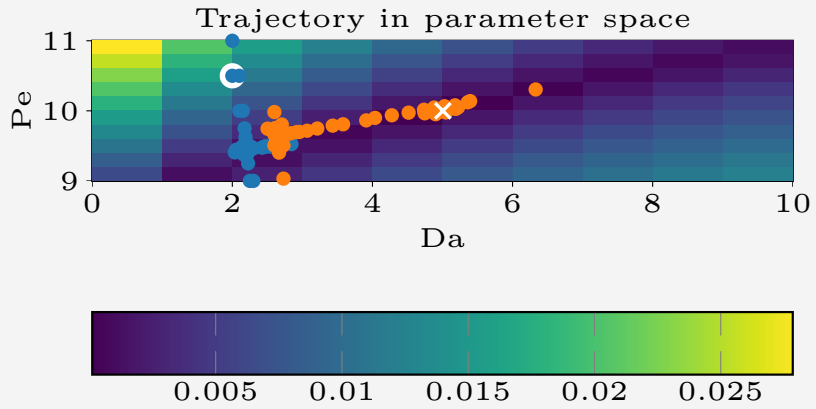
Components of the adaptive model:

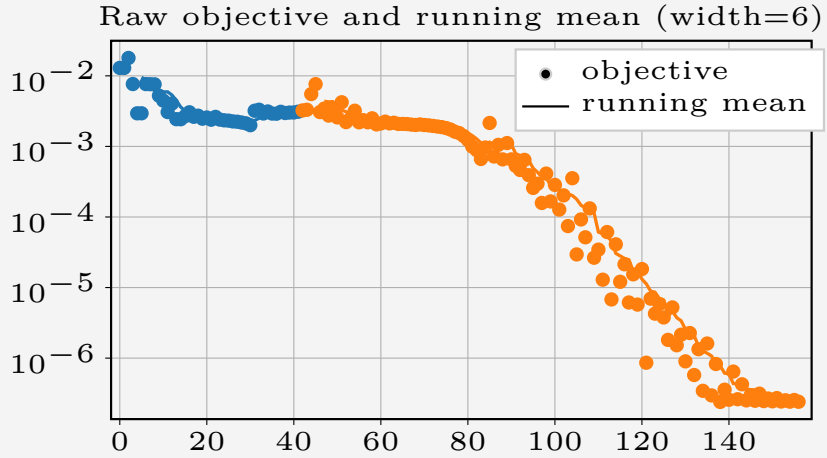
- FOM: FE grid with $N_h = 2{,}051{,}841$ DoFs, $K = 10{,}001$ time steps
- RB-ROM: **H**ierarchical **a**pproximate **P**roper **O**rthogonal **D**ecomposition (HaPOD) [Himpe/Leibner/Rave'18]

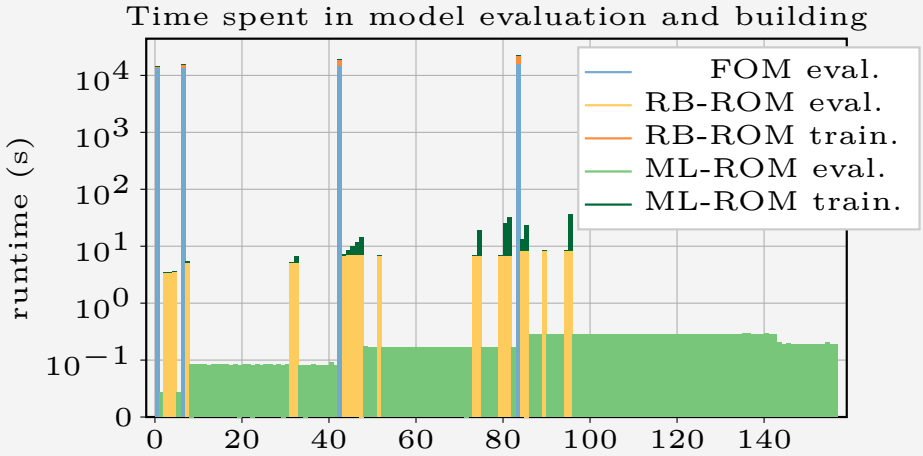


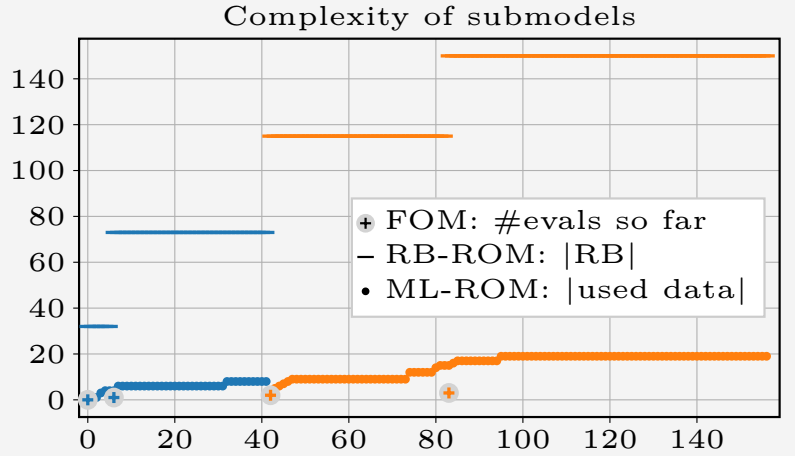
- MLM: Time-"vectorized" approach with **V**ectorial **K**ernel **O**rthogonal **G**reedy **A**lgorithm (VKOGA) [Santin/Haasdonk'21]

Numerical experiments I – PDE-constr. optimization







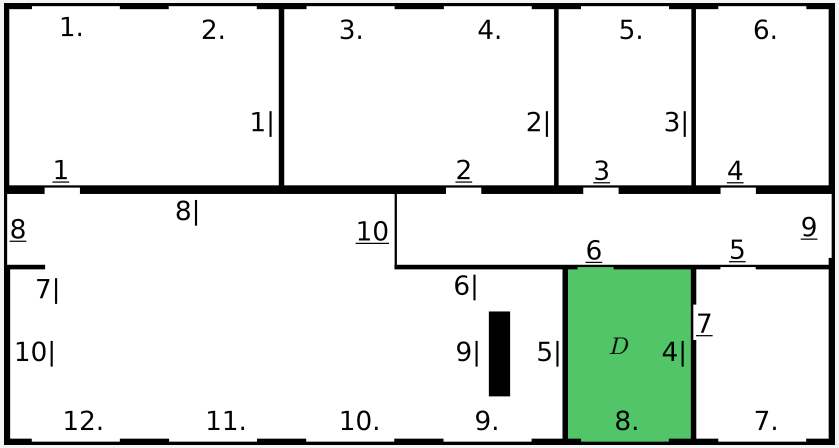


Numerical experiments II – Monte Carlo

Parameter-dependent bilinear form a and source term l:

$$a(u, v; \mu) = \int_\Omega \kappa(\mu)\, \nabla u(x) \cdot \nabla v(x)\, \mathrm{d}x,$$

$$l(v; \mu; t) = \int_\Omega v\, \ell(\mu; t)\, \mathrm{d}x.$$



Numerical experiments II – Monte Carlo

Parameter-dependent bilinear form a and source term l:

$$a(u, v; \mu) = \int_\Omega \kappa(\mu)\, \nabla u(x) \cdot \nabla v(x)\, \mathrm{d}x,$$

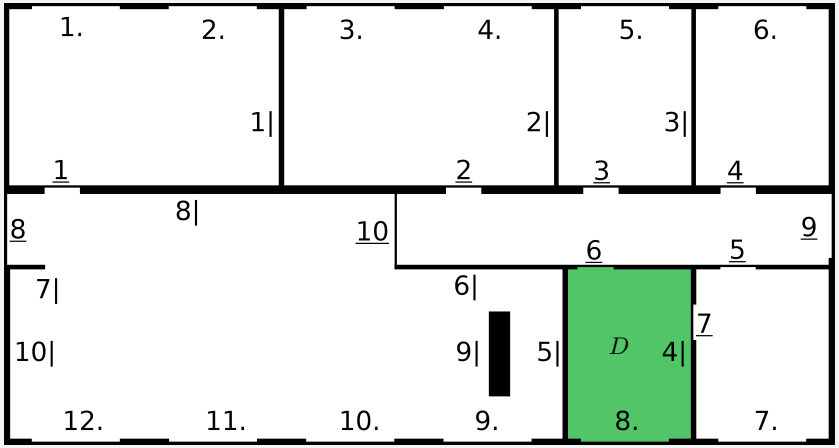
$$l(v; \mu; t) = \int_\Omega v\, \ell(\mu; t)\, \mathrm{d}x.$$

Quantity of interest at time $t \in [0, T]$:

$$f(\mu; t) := \frac{1}{|D|} \int_D u(t, x; \mu)\, \mathrm{d}x$$

Average over time interval $\tau \subset [0, T]$:

$$\bar{f}(\mu) := \frac{1}{|\tau|} \int_\tau f(\mu; t)\, \mathrm{d}t$$



Numerical experiments II – Monte Carlo

Expectation and variance of $\bar{f}$ with respect to density $\rho\colon \mathcal{P} \to [0, \infty)$:

$$\mathrm{E}[\bar{f}] := \int_{\mathcal{P}} \rho(\mu)\bar{f}(\mu)\,\mathrm{d}\mu, \qquad \mathrm{Var}[\bar{f}] := \int_{\mathcal{P}} \rho(\mu)\left(\bar{f}(\mu) - \mathrm{E}[\bar{f}]\right)^2 \mathrm{d}\mu$$

Numerical experiments II – Monte Carlo

Expectation and variance of $\bar{f}$ with respect to density $\rho\colon \mathcal{P} \to [0,\infty)$:

$$\mathrm{E}[\bar{f}] := \int_{\mathcal{P}} \rho(\mu)\bar{f}(\mu)\,\mathrm{d}\mu, \qquad \mathrm{Var}[\bar{f}] := \int_{\mathcal{P}} \rho(\mu)\left(\bar{f}(\mu) - \mathrm{E}[\bar{f}]\right)^2 \mathrm{d}\mu$$

Monte Carlo estimation of $\mathrm{E}[\bar{f}]$ and $\mathrm{Var}[\bar{f}]$:

$$\mathrm{E}[\bar{f}] \approx \hat{\theta}_{\bar{f}} := \frac{1}{N_{\mathrm{mc}}} \sum_{\mu\in\mathcal{P}_{\mathrm{mc}}} \bar{f}(\mu),$$

$$\mathrm{Var}[\bar{f}] \approx \frac{1}{(N_{\mathrm{mc}}-1)} \sum_{\mu\in\mathcal{P}_{\mathrm{mc}}} \left(\bar{f}(\mu) - \hat{\theta}_{\bar{f}}\right)^2,$$

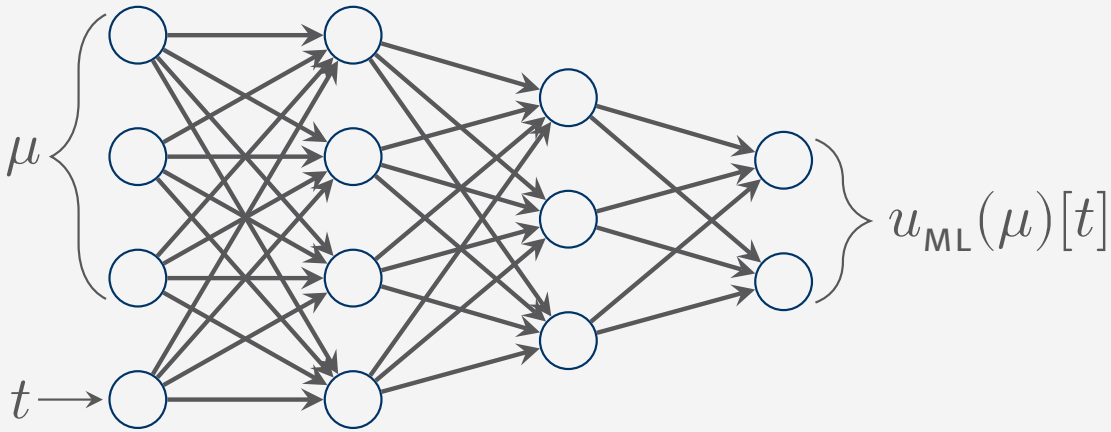
where $\mathcal{P}_{\mathrm{mc}} \subset \mathcal{P}$ is randomly sampled according to ρ.

Numerical experiments II – Monte Carlo

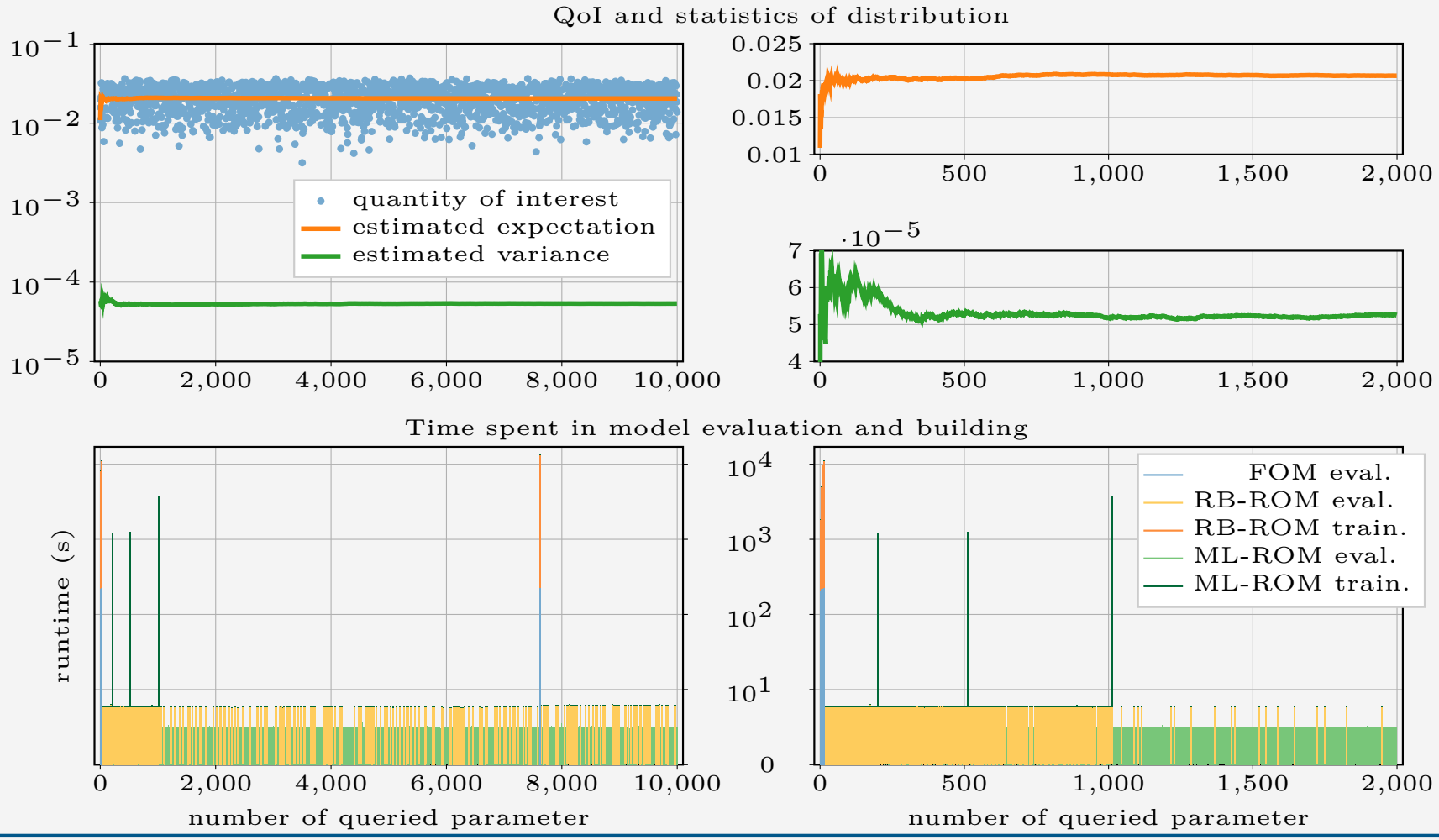
Components of the adaptive model:

- FOM: FE grid with $N_h = 321{,}206$ DoFs, $K = 1000$ time steps
- RB-ROM: HaPOD
- MLM: “Random-access”-in-time approach with Deep Neural Network (training only after 200 new ROM solutions are available)

  [Wang/Hesthaven/Ray’19]



Numerical experiments II – Monte Carlo



Thank you for your attention!

For more details, see:

B. Haasdonk, H. Kleikamp, M. Ohlberger, F. Schindler, T. Wenzel, *A new certified hierarchical and adaptive RB-ML-ROM surrogate model for parametrized PDEs*, arXiv, (2022), https://arxiv.org/abs/2204.13454.

References I

M. Grepl and A. Patera, *A posteriori error bounds for reduced-basis approximations of parametrized parabolic partial differential equations*, ESAIM: Mathematical Modelling and Numerical Analysis, 39 (2005), pp. 157–181, https://doi.org/10.1051/m2an:2005006.

Q. Wang, J. S. Hesthaven, and D. Ray, *Non-intrusive reduced order modeling of unsteady flows using artificial neural networks with application to a combustion problem*, J. Comput. Phys., 384 (2019), pp. 289–307, https://doi.org/10.1016/j.jcp.2019.01.031.

G. Santin and B. Haasdonk, *Kernel methods for surrogate modeling*, in Model Order Reduction, P. Benner, S. Grivet-Talocia, A. Quarteroni, G. Rozza, W. Schilders, and L. M. Silveira, eds., vol. 2, De Gruyter, 2021, pp. 311–353.

References II

C. Himpe, L. Leibner and S. Rave, *Hierarchical approximate proper orthogonal decomposition*, in SIAM Journal on Scientific Computing, vol. 40, 2018, pp. A3267–A3292.